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# Love-type waves in layered systems consisting of two cubic piezoelectric crystals

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In memory of Prof. Dr. Galina Georgievna Kessenikh

**Abstract**

Dispersion relations of the seven partial Love-type waves (LTW7) have been found numerically for two-layer systems consisting of the class-23 cubic piezoelectric media $Bi_{12}SiO_{20}$ and $Bi_{12}GeO_{20}$, for two cases: a layer of $Bi_{12}SiO_{20}$ on a substrate of $Bi_{12}GeO_{20}$, and the reverse configuration. A few modes of LTW7 waves are shown, the first of which begins at a threshold value of $kh^{\mathrm{th}} \sim 5.3$. The values of $kh^{\mathrm{th}}$ for the classical Love waves are tabulated for comparison with the LTW7 waves. "Dispersive solutions" have also been found, whose phase speeds are higher than the bulk shear wave speeds in either medium.


## 1. Introduction

Layered structures with inhomogeneous boundary conditions, for example, a thin film on a substrate, are currently of interest. The important thing is to know phase velocities and dispersion relations, for applications in filters and acoustic delay lines. In 1911, Love [1] analyzed a layered system consisting of an isotropic thin film on an isotropic substrate, solid-coupled at their interface. He concluded that shear surface waves localized in the thin film and decaying in the substrate can exist if the velocity of the bulk shear wave in the thin film is less than that in the substrate. These shear surface waves are now known as the Love waves; their polarization is

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perpendicular to the sagittal plane formed by both the normal to the interface of a medium and the wavevector in the direction of wave propagation. Interest was later shown in the possible existence of waves with the same polarization in piezoelectric, anisotropic layered systems [2] for applications to delay lines, filters, etc., and the waves were called "pure" Love-type waves (LTWs). Such "pure" LTWs can exist in layered systems only in special so-called highly symmetric directions of wave propagation, for example, if the sagittal plane is perpendicular to an odd-order symmetry axis. It was also noted in Ref. [2] that finding the dispersion relation of these waves is very complicated numerically. But in particular cases, for example, the so-called transversal-isotropic cases treated in Refs. [3,4], LTW waves can be studied analytically. In Ref. [3] the surface waves of Love-type for systems of an isotropic layer on a piezoelectric substrate consisting of either the hexagonal (the classes 6, 622, 6 mm) or the tetragonal (the classes 4, 422, 4 mm) monocrystals were analytically treated and in Ref. [4] vice versa: a piezoelectric layer consisting of material of the same classes on an isotropic substrate. Also the transversal-isotropic case was discussed in Ref. [5], where a CdS piezoelectric thin film of class 6 mm covers isotropic substrates. Dispersion relations for the layered systems can be numerically obtained.

In this paper, results concerning the numerical study of the layered systems are reported, for the case when both the layer and the substrate are piezoelectric cubic crystals $Bi_{12}SiO_{20}$ and $Bi_{12}GeO_{20}$ of class 23, taking into account the piezoeffect for both media. It is thought that such layered systems can be readily manufactured.

## 2. Description of the problem

Today, it is well understood that bulk shear waves in piezoelectric bulk monocrystals are not bulk waves, but the surface Bleustein–Gulyaev (BG) waves [6,7] with polarization perpendicular to the sagittal plane. In the case when a piezoelectric thin film covers a piezoelectric bulk crystal, the LTWs can probably exist. Layered systems, in which either a substrate in Refs. [3,8] or a thin film in Ref. [4] is a piezoelectric (either tetragonal or hexagonal) crystal with a second isotropic medium, were analytically studied, and possible changes were shown in the modes of the LTWs due to the piezoeffect for the transversal-isotropic case. The analytical study of layered systems of a piezoelectric layer on a piezoelectric substrate is very complicated, even for the transversal-isotropic cases.

Principles of investigations of dispersive surface waves in layered piezoelectric media are written in detail in Refs. [2,9]. First of all, it is necessary to find the complete displacements and complete electrical potential for each medium, separately using material constants for each medium: densities $\rho$, elastic $C_{ijkl}$ and piezoelectric $e_{ijk}$ constants, dielectric coefficients $\varepsilon_{ij}$, and solving propagation equations. For the free space, the dielectric coefficient $\varepsilon_0$ is taken. This part of the calculation is like the one on the investigations of surface waves in piezoelectric bulk monocrystals. Details about this one can also be found in Refs. [10,11]. However, the differences of the investigations between the bulk medium and the layered medium are in the boundary condition determinants (BCDs). For layered media [2,9], the BCD of thirteenth order (taking into account the piezoeffect for both the layer and the substrate) is a complex number, and there will be solutions of the phase velocity, if the BCD13 falls to zero. The BCD will be ninth order, BCD9, without taking into account the piezoeffect for centrosymmetrical crystals. Numerically, it means to find the minima of the BCD13. In the highly symmetric cases, described in Refs. [2,9], the BCD13 can be written as two BCDs, either the BCD7 of seventh order for the piezo-electromechanical waves of Love-type (LTW7) and the BCD6 of sixth order for the mechanical waves of Rayleigh type (RTW6), or the BCD3 of third order for the mechanical waves of LTWs (LTW3) and the BCD10 of tenth order for the piezoelectromechanical waves of Rayleigh type (RTW10). They are "pure" waves of Love-type and Rayleigh type, which can be treated separately for simplicity. Of the classical three-partial Love waves (LW3) in isotropic media, one can read Ref. [10].

## 3. Theory

Let us treat the layered system shown in Fig. 1 on the wave propagation direction, in which the sagittal plane is perpendicular to an odd-order symmetry axis for both treated media. Therefore, for such waves, polarized along the $x_2$-axis and perpendicular to the sagittal plane as well, only three independent components of the modified Green–Christoffel tensor are treated, taking into account the piezoelectric effect: $GL_{22}$, $GL_{42} = GL_{24}$, $GL_{44}$. The displacement $U_2$ along the $x_2$-axis and the electrical potential $\varphi$ in view of plane waves are

$$U_2 = u \exp[\mathrm{j}k(n_1x_1 + n_3x_3 - Vt)],$$
$$\varphi = \phi \exp[\mathrm{j}k(n_1x_1 + n_3x_3 - Vt)], \tag{1}$$

where $\mathrm{j} = (-1)^{1/2}$, $u$ and $\phi$ are the corresponding amplitudes, $k$ is the wavenumber in the direction of wave propagation, and $V = \omega/k$ is the phase velocity. The coupled equations of motion can be taken in the following view:

$$\rho\frac{\partial^2 U_2}{\partial t^2} = C_{44}\left(\frac{\partial^2 U_2}{\partial x_1^2} + \frac{\partial^2 U_2}{\partial x_3^2}\right) + 2e_{14}\frac{\partial^2 \varphi}{\partial x_1 \partial x_3},$$
$$0 = 2e_{14}\frac{\partial^2 U_2}{\partial x_1 \partial x_3} - \varepsilon_{11}\left(\frac{\partial^2 \varphi}{\partial x_1^2} + \frac{\partial^2 \varphi}{\partial x_3^2}\right), \tag{2}$$

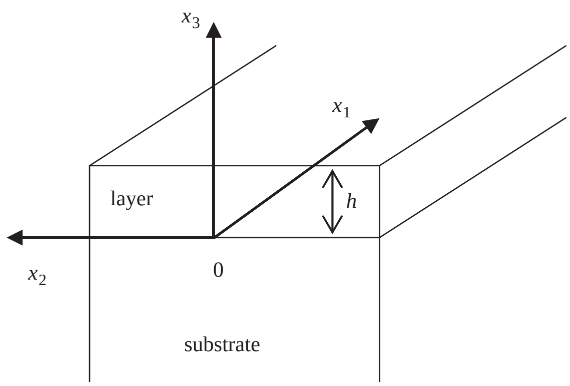


Fig. 1. The coordinate system of the layered system, where $h$ is the layer thickness.

which correspond to waves with such polarization for the treated cubic materials. Eq. (2) is obtained from the common equations of motion for piezoelectric materials, which are given in Refs. [10,11], after straightforward transformations, which are applied for the treated case as well.

Therefore, the system of two homogeneous equations is written as follows:

$$C[(1+n_3^2)-(V/V_t)^2]u+2en_3\phi=0,$$
$$2en_3u-\varepsilon(1+n_3^2)\phi=0, \tag{3}$$

where $V_t=(C/\rho)^{1/2}$ is the velocity of the bulk shear wave, $C=C_{44}=C_{55}=C_{66}$ is the corresponding non-zero component of the elastic constants tensor, $e=e_{14}=e_{25}=e_{36}$ is the single non-zero component of the piezoelectric constants tensor, $\varepsilon=\varepsilon_{11}=\varepsilon_{22}=\varepsilon_{33}$ is the single component of material tensor of the dielectric constants; $\rho$ is the material density. About the physical properties of crystals and their representations by tensors, one can read Ref. [12]. In Eqs. (1) and (3), there are directional cosines $n_1=1, n_2=0, n_3=n_3$. For the free space, in the equation set (3), there is only one non-zero component $\varepsilon_0$ of the dielectric permittivity tensor.

Expanding the determinant formed by the coefficients before the amplitudes $u$ and $\phi$ in the equation set (3), there appears a secular cubic polynomial equation for determination of four polynomial roots:

$$n^2-Bn-K^2=0 \quad \text{with } n=1+n_3^2. \tag{4}$$

Therefore, the polynomial roots $n_3^{(m)}$ are as follows:

$$n_3^{(m)}=\pm\sqrt{-1+B/2\pm\sqrt{B^2+4K^2}/2}, \tag{5}$$

where $m=1,2,3,4$, but $B=(V/V_t)^2-K^2$. Here $K^2=4e^2/C\varepsilon$ is the coefficient of electromechanical coupling (CEMC). Expression (5) shows dependence of the $n_3^{(m)}$ on the phase velocity $V$. From the second equation of the equation set (3), one can determine the electrical potential amplitudes $\phi^{(m)}$ as a function of the phase velocity $V$:

$$\phi^{(m)}=(2e/\varepsilon)n_3^{(m)}/(1+(n_3^{(m)})^2). \tag{6}$$

In expression (6), the corresponding displacement amplitudes $u^{(m)}$ are taken to be equal to unity.

The complete displacement $U$ and the complete electrical potential $\Phi$ are functions of the eigenvalues $n_3^{(m)}$ and of the eigenvectors ($u^{(m)}$, $\phi^{(m)}$):

$$U=\sum_m f^{(m)}u^{(m)}\exp[jk(n_1x_1+n_3^{(m)}x_3-Vt)],$$
$$\Phi=\sum_m f^{(m)}\phi^{(m)}\exp[jk(n_1x_1+n_3^{(m)}x_3-Vt)], \tag{7}$$

where $f^{(m)}$ are called the unknown amplitudes. In expression (7), the index $m$ runs from 1 to 4 for a layer but $m=1,2$ for a substrate.

In Eq. (5), it is clearly seen that four polynomial roots can be either all imaginary ones (for $V<V_t$) or two real and two imaginary ones (for $V>V_t$). A situation with all four real roots is not possible. According to expression (5), there is also the third possibility for the roots, such as two trivial and two imaginary roots for $V = V_t$:

$$n_3^{1,2} = 0,$$
$$n_3^{3,4} = \pm \mathrm{j}\sqrt{1 + K^2}. \quad (8)$$

The two trivial roots correspond to the bulk shear waves. In reality, the condition is always fulfilled such as $K^2 < 1$, even $K^2 \ll 1$, therefore $K < 1$ as well. For example, $K^2(Bi_{12}SiO_{20}) \sim 0.565$ and $K^2(Bi_{12}GeO_{20}) \sim 0.509$, but $K^2(GaAs) \sim 0.016$ according to Ref. [13]. Thus, for the phase velocity $V \to +\infty$ ($V > V_t$), the roots can be represented in the following view:

$$n_3^{1,2} \to \pm\sqrt{\left(\frac{V}{V_t}\right)^2 - 1},$$
$$n_3^{3,4} \to \pm \mathrm{j}\sqrt{1 + K^2}. \quad (9)$$

For two real roots in Eq. (9), it is noted that taking $V \sim 10V_t$ there are absolute values of the real roots, which are only one order greater than the ones of the imaginary roots in Eq. (9).

But for the case $B = 0$ ($V < V_t$ owing to the condition $K^2 < 1$), one gets

$$n_3^{1,2,3,4} = \pm \mathrm{j}\sqrt{1 \mp K}. \quad (10)$$

On the other hand, the second limit for all imaginary roots can be found from expression (5), substituting the phase velocity $V = 0$ ($V \to 0$) that gives

$$n_3^{1,2,3,4} = \pm \mathrm{j}\sqrt{1 + K^2/2 \mp K(1 + K^2/4)^{1/2}}. \quad (11)$$

For weakly piezoelectric materials, taking into account the condition $K^2 \ll 1$ and leaving only term $K$ under square root in expression (11), there are four imaginary roots, the values of which are close to the ones in expression (10):

$$n_3^{1,2,3,4} \to \pm \mathrm{j}\sqrt{1 \mp K}. \quad (12)$$

Therefore, for all cubic weakly piezoelectric materials in the wide range of the phase velocity, $0 \leq V \leq V_t$, in which surface waves can exist, it is fulfilled that the absolute values of the corresponding two negative imaginary roots increase from their minimal values in expression (8) up to their maximal ones in expressions (10)–(12).

Two negative roots are taken for a substrate in order to have wave damping, while for a thin layer all four roots are taken. For a layer and a substrate in Eqs. (1)–(7), there appear corresponding components of the material tensors and the corresponding densities.

It is now necessary to briefly discuss the seven boundary conditions, treating the LTW7 waves, which consist of both the electrical and mechanical parts of the ones both at $x_3 = 0$ and $x_3 = h$ (see Fig. 1). The boundary conditions at $x_3 = 0$ are: continuity of both the corresponding mechanical displacement and the corresponding stress tensor component, and continuity of both the electrical potential and the normal component of the electrical displacements. The boundary conditions at $x_3 = h$ are: equality to zero of the corresponding stress tensor component, and continuity of both the electrical potential and the normal component of the electrical displacements.

Suitable phase velocities will be found, if the seven-order boundary conditions determinant (BCD7) falls to zero. BCD7 is formed from the boundary conditions by (7 × 7)-coefficient factors for the seven unknown amplitudes $f^{(M)}$: two of which are related to a substrate, four correspond to a layer, but the seventh one is reserved for the free space. The unknown amplitudes $f^{(M)}$, which are also called weight factors, can be readily calculated for each suitable phase velocity from each other, taking one of those as the known one. The coefficients are functions of the material constants and of the phase velocity $V$ as well.

## 4. Numerical results

In this numerical experiment, two layered systems are treated: the layer of $Bi_{12}SiO_{20}$ on the substrate of $Bi_{12}GeO_{20}$, and vice versa, the layer of $Bi_{12}GeO_{20}$ on the substrate of $Bi_{12}SiO_{20}$. Waves propagate in the direction along the $x_1$-axis perpendicular to the symmetry axis of the second order for both treated media, as shown in Fig. 1. Waves are localized in the thin layer of thickness $h$ with damping in the direction of the negative values of the $x_3$-axis. The LTW7 waves can exist in the direction of wave propagation perpendicular to the second-order symmetry axis for the treated media of the non-centrosymmetrical class 23. Therefore, it will be seven partial waves similar to the transversal-isotropic case [8]. The material constants $C_{ijkl}$, $e_{ijk}$ and $\varepsilon_{ij}$ for both piezoelectric materials can be chosen, for example, from Refs. [13,14].

The dispersion relations of the phase velocity dependence of the LTW7 waves, taking into account the piezoeffect for both media on non-dimensional value of $kh$, where $k$ is the wavenumber in the direction of wave propagation and $h$ is the layer thickness, are shown in Fig. 2a and b. The phase velocity of shear surface waves for bulk piezoelectric crystals can be written

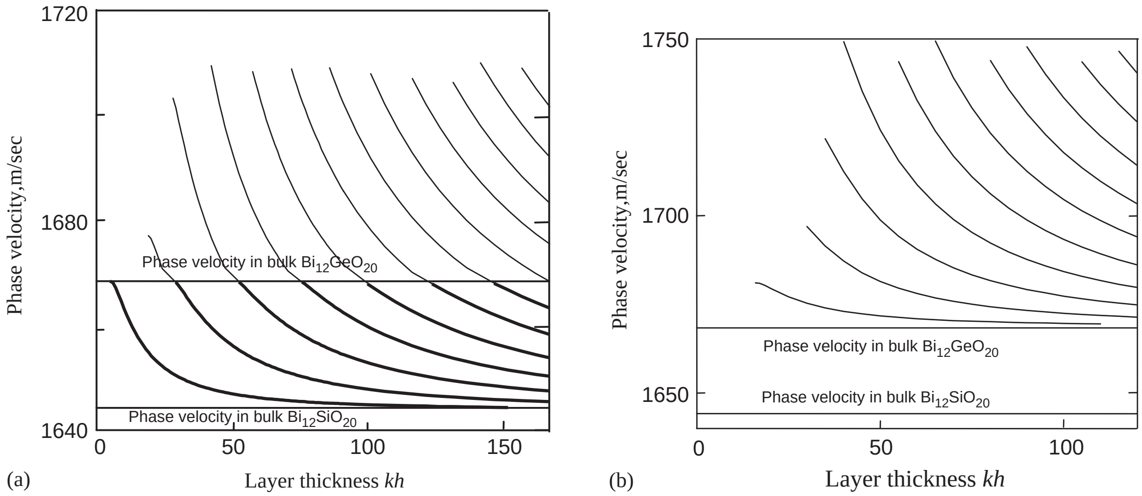


Fig. 2. The dispersion relations. (a) Seven modes of the dispersive LTW7 waves are shown by bold solid lines. The "dispersive solutions" are shown by simple solid lines situated above the corresponding modes of the LTW7 waves. (b) Here, the LTW7 waves cannot exist, but the "dispersive solutions" exist.

as $V \sim V_{ph0}(1+K_D^2)^{1/2}$, where $V_{ph0} = (C_{44}/\rho)^{1/2}$ and $K_D^2$ is the so-called CEMC. In layered systems, the coefficient $K_D^2$ depends on the layer thickness $kh$ and is called the dynamic CEMC, which was introduced in Refs. [3,4,8] for convenience. Fig. 2a represents the dispersion relation for the layered system consisting of the layer of $Bi_{12}SiO_{20}$ on the substrate of $Bi_{12}GeO_{20}$. As it is seen, the first mode of the LTW7 waves begins in this case at $kh > 5.3$, but not at $kh = 0$, in comparison with the classical three-partial Love waves (LW3) in isotropic media. In Table 1, for comparison, seven modes of both the classical Love waves (without taking into account the piezoeffect for both the layer and the substrate) and the LTW7 waves for treated media are shown. In this case, for treated cubic piezoelectric crystals, the influence of the piezoeffect is similar to the case treated in Ref. [3] for an isotropic layer on a transversal-isotropic substrate of crystals of classes 622, 422, where for the first mode, the so-called "silence zone" [3] is present and the dynamic CEMC is negative (CEMC < 0).

All modes of the LTW7 waves in Fig. 2a are in the phase velocity range between the phase velocity of the bulk shear wave in $Bi_{12}SiO_{20}$ ($V_{ph1}$) and the one in $Bi_{12}GeO_{20}$ ($V_{ph2}$). Probably, all modes of the LTW7 waves are related to the second type of the waves, because the first mode of the LTW7 waves begins at $kh \sim 5.3$, but not at $kh = 0$. Therefore, the first mode of the LTW7 waves can be the second-type waves, but not the first-type ones, or it is possible to say that there is no first mode of the waves and the modes begin with number 2 (see in Ref. [2] about waves of the first and second types). Possibly, the LTW7 waves of the first type, beginning at $kh = 0$, exist in such directions of wave propagation, where the surface Bleustein–Gulyaev waves can propagate. Different sectors of the existence of the surface BG waves were studied in Ref. [15], see also Ref. [16].

Also, it is very surprising to find "dispersive solutions" for the phase velocity, which are greater than the value of the phase velocity $V_{ph2}$ of the bulk shear wave for $Bi_{12}GeO_{20}$. These dispersive solutions can correspond to a new type of dispersive leaky waves with polarization, like the one of the surface LTWs. The solutions are continuations of corresponding high modes $(2, 3, \ldots)$ of the LTW7 waves above the phase velocity $V_{ph2}$ in the bulk crystal $Bi_{12}GeO_{20}$. At $kh \to \infty$, the LTW7 waves approach the phase velocity $V_{ph1}$ in the bulk crystal $Bi_{12}SiO_{20}$. These solutions correspond to local minima of the BCD7, that is the usual thing for leaky waves, but not to global ones, which are solutions for both surface and bulk waves. In this case, the local ones of the BCD7 do not fall to zero; therefore, the solutions are not true solutions, but some experimentalists believe that such dispersive leaky waves can be experimentally excited. These "dispersive solutions" correspond to

Table 1
The values of $kh^{th}$

| Mode $N^0$ | The values of $kh^{th}$ (LW3 waves) | The values of $kh^{th}$ (LTW7 waves) |
|---|---|---|
| 1 | 0.0 | 5.30 |
| 2 | 17.76 | 28.24 |
| 3 | 35.51 | 51.18 |
| 4 | 53.27 | 74.12 |
| 5 | 71.03 | 97.06 |
| 6 | 88.79 | 120.0 |
| 7 | 106.5 | 142.9 |

the taken negative roots for the treated substrates: one imaginary and one real root. If a positive real root is taken instead of a negative one, such "dispersive solutions" are also found.

Fig. 2b represents the dispersion relation for the layered system consisting of the layer of $Bi_{12}GeO_{20}$ on the substrate of $Bi_{12}SiO_{20}$. For this layered system, the phase velocity $V_{ph2}$ for the layer is greater than the one $V_{ph1}$ for the substrate, and there are no solutions in the velocity range between $V_{ph1}$ and $V_{ph2}$. It means that this is similar to the classical three-partial Love waves (LW3) in isotropic media, where the LW3 waves can exist in the phase velocity range between bulk shear waves $V_{01}$ and $V_{02}$, if $V_0$ for an isotropic layer is less than the one for an isotropic substrate. Also, the phase velocity solutions above the phase velocity $V_{ph2}$ in $Bi_{12}GeO_{20}$ are present in this layered system as well, and these "dispersive solutions" (which could be the new type of the leaky waves) approach the phase velocity $V_{ph2}$ at $kh \to \infty$. It is possible to find a short abstract about it in Ref. [17] in Russian, and also see Ref. [18].

In the famous book Springer Series on Wave Phenomena [16], surface (interfacial) inhomogeneities on the surface of monocrystals (isotropic media as well), which play the role of a very thin additional "softer" layer on the surface, and cause changes in the characteristics of acoustic waves in monocrystals, were considered. For example, the problems of surface acoustic wave interaction with periodic topographic gratings, widely used in filters and resonators, are under careful consideration. The most important results of surface wave scattering by local defects such as grooves, random roughness, and elastic wedges are given. Different theoretical approaches and practical rules for solving the surface wave problems are presented. But in Ref. [19], the theoretical analysis of Bleustein–Gulyaev surface acoustic wave propagation in a prestressed layered piezoelectric structure were described, and numerical calculations were performed for the case, where both the layer and the substrate are identical $LiNbO_3$, except that they are polarized in opposite directions. It results in an almost linear behavior of the relative change in phase velocity versus the initial stress, and, therefore, possible applications in the design of acoustic wave devices were suggested. Some of the problems can be met in real experiments investigating manufactured two-layer systems, two of which are theoretically studied in the present work.

In the review paper [20] were presented general considerations about physical reasons for the existence of surface acoustic waves and, in particular, for different types of shear surface acoustic waves. But in the more recent review [21] concerning shear-horizontal-type waves, attention was paid to the relationship between the so-called surface skimming bulk waves (SSBW) and the so-called surface Bleustein–Gulyaev–Shimizu waves (BGShW) in monocrystals, in particular, the phase velocities of those waves coincide. But in Refs. [22,23], the investigations were done on LTWs, as well as leaky surface acoustic waves (LSAW) consisting of isotropic $Ta_2O_5$ (or $SiO_2$) layer on Langasite (or Quartz) substrate. Both theoretical calculations and experimental measurements of the phase velocity $V_{ph}$ were also presented, only for the first mode, with notation that LSAW waves become the surface LTW waves. Unfortunately, only several experimental points for the phase velocity were shown, with which it is impossible to have a true picture about approximation of the LSAW mode to the bulk shear wave for the substrates. The LSAW mode looks like a continuation of the LTW mode. It was also mentioned that for $Bi_{12}GeO_{20}$/Y–X–$LiNbO_3$, there was discontinuity of those modes.

The results, shown in Fig. 2a and b of the present paper, allow the discussion that the series of the "dispersive solutions" is owing to the material properties, but not due to a relationship between the "dispersive solutions" (leaky waves) and the LTW7 waves, because the solutions exist in the layered system in Fig. 2b, where the LTW7 waves cannot propagate.

Table 1 shows the threshold values of $kh^{\text{th}}$ for the beginning modes both for the classical LW3 waves and for the LTW7 waves. The values of $kh^{\text{th}}$ for the LW3 waves were calculated with the formula $kh^{\text{th}} = n_0\pi/[(V_S/V_L)^2 - 1]^{1/2}$ [24], where $n_0 = 0, 1, 2, \ldots$ and $V_S$, $V_L$ are the phase velocities of the bulk shear waves for the substrate and layer, respectively. The values of $kh^{\text{th}}$ for the LTW7 waves were taken from Fig. 2a. Therefore, it is possible to write that the influence of the piezoeffect on the modes of the LTW3 waves causes a shift of all the LTW3 modes from the first to the last mode, like the first seven modes shown in Table 1. In addition, it is clearly seen that the beginning modes of the LTW7 waves are equidistant from each other, but not from the corresponding ones of the classical LW3 waves. On the other hand, the influence of the piezoeffect for layered systems consisting of piezoelectrics of classes 23 and $\bar{4}32$ can show the existence of a single mode of dispersive Bleustein–Gulyaev–Love-type waves, probably, confined between two corresponding BG waves in the propagation directions, in which the BG waves can propagate. The BG waves exist in [1 0 1] direction of wave propagation for the treated materials, which can be the next subject for research. However, the interesting thing is to investigate the case when the BG wave can exist only in either a layer or a substrate.

## 5. Conclusions

The numerically obtained dispersion relations of the LTW7 waves for the treated layered systems consisting of cubic piezoelectric crystals $Bi_{12}SiO_{20}$ and $Bi_{12}GeO_{20}$ of class 23 have shown that the LTW7 waves can exist in the phase velocity range between the bulk shear wave $V_{\text{ph1}}$ in bulk $Bi_{12}SiO_{20}$ and the one $V_{\text{ph2}}$ in $Bi_{12}GeO_{20}$, if the phase velocity for the substrate is greater than the one for the layer. In the layered system, in which the phase velocity for the substrate is less than the one for the layer, the LTW7 waves cannot exist for the treated case. Also "dispersive solutions" of the phase velocity were numerically found, which are situated above the phase velocity range between $V_{\text{ph1}}$ and $V_{\text{ph2}}$. Also, it is possible to conclude that the "dispersive solutions" are either properties of the BCD7 or the ones of the layered systems consisting of the piezoelectric materials that can be used.

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